Index

Original Investigations and Short Communications

Ahlrichs, R. see Ehrhardt, C. 231
Baker, J.: Classical chemical concepts from *ab initio* SCF calculations 221
Bénière, F., see Morton-Blake, D. A., et al. 389
Bonaccorsi, R., see Cammi, R., et al. 271
Bonačić-Koutecký, V., Michl, J.: Photochemical *syn-anti* isomerization of a Schiff base: A two-dimensional description of a conical intersection in formaldimine 45
Braga, M., see Larsson, S. 291
Brocas, J.: Comments on characteristic polynomials of chemical graphs 155
Brown, F. B., Schwenke, D. W., Truhlar, D. G.: An *ab initio* potential energy surface and dynamics calculations for vibrational excitation of I_2 by He 23
Burke, L. A.: The influence of the cyclic product's structure on the Diels-Alder transition state .. 101
Cammi, R., Bonaccorsi, R., Tomasi, J.: Counterpoise corrections to the interaction energy components in bimolecular complexes 271
Chiu, Y.-N., Wang, F. E.: Symmetry-adapted cluster *f*-orbitals and a vector method for generally oriented *f*-orbital overlaps 179
Ciosłowski, J.: Additive nodal increments for approximate calculation of the total π-electron energy of benzenoid hydrocarbons 315
Contreras, R. H., see Gavarini, H. O., et al. 171
Corish, J., see Morton-Blake, D. A., et al. 389
Dailey, W. P., see Orendt, A. M., et al. 421
Davidson, E. R., see Feller, D. 57
Deb, B. M., see Gosh, S. K. 336
Dias, J. R.: Properties and derivation of the fourth and sixth coefficients of the characteristic polynomial of molecular graphs — New graphical invariants 107
Ehrhardt, C., Ahlrichs, R.: Population analysis based on occupation numbers. II. Relationship between shared electron numbers and bond energies and charcterization on hypervalent contributions 231
Elbert, S. T., see Schmidt, M. W., et al. 69
Facelli, J. C., see Orendt, A. M., et al. 421
Feller, D., Davidson, E. R.: Difficulties in *ab initio* CI calculations of the hyperfine structure of small radicals 57
Fernández, A.: Jahn—Teller distortion motions as separatrices in PES 285
Gama, A. A. S. da: Donor acceptor interaction in metalloproteins 159
Gavarini, H. O., Natiello, M. A., Contreras, R. H.: A polarization propagator analysis of the geminal ^{31}P—^{31}P coupling in bis(difluorophosphino)amine 171
Giambiagi, M., see Giambiagi, M. S. de, et al. 337
Giambiagi, M. S. de, Giambiagi, M., Jorge, F. E.: Bond index: relation to second-order density matrix and charge fluctuations 337
Goodisman, J.: Conduction electrons of the metal in the electrochemical interface 197
Gopinathan, M. S., see Jug, K. 343
Gosh, S. K., Deb, B. M.: A density-functional calculation of dynamic dipole polarizabilities of noble gas atoms (Corrigendum) 336
Grant, D. M., see Orendt, A. M., et al. 421
Handy, N. C., Knowles, P. J., Somasundram, K.: On the convergence of the Møller-Plesset perturbation series 87
Hao, Z.-D., see Koga, T., et al. 211
Ishenko, S. Ia., Vener, M. V., Mamaev, V. M.: Two-dimensional model of intramolecular hydrogen bond 351

Jorge, F. E., see Giambiagi, M. S. de, et al. ... 337
Jug, K., Gopinathan, M. S.: Valency changes in chemical reactions ... 343
King, R. B.: Chemical applications of topology and group theory. 17. An information theoretical approach to polyhedral symmetry (1) ... 143
Kirtman, B., see Maclagan, R. G. A. R. ... 407
Knowles, P. J., see Handy, N. C., et al. ... 87
Koga, T., Nakao, R., Hao, Z.-D.: Diatomic interactions in momentum space. Bond polarity ... 211
Kutzelnigg, W., see Orendt, A. M., et al. ... 421
Kutzelnigg, W.: r_{12}-Dependent terms in the wave function as closed sums of partial wave amplitudes for large l ... 445
Lam, B., see Schmidt, M. W.,et al. ... 69
Larsson, S., Braga, M.: Atomic charges based on spherical harmonics expansion at the atomic centers ... 291
Maclagan, R. G. A. R., Kirtman, B.: Factors determining bond angles from a classical valence bond perspective. Covalent structure of H_2O ... 407
Makarewicz, J.: Adiabatic multi-step separation method and its application to coupled oscillators ... 321
Mamaev, V. M., see Ishenko, S. Ia., et al. ... 351
Michl, J., see Bonačić-Koutecký, V. ... 45
Michl, J., see Orendt, A. M., et al. ... 421
Miller, W. H., see Shi, S. ... 1
Morton-Blake, D. A., Corish, J., Bénière, F.: A molecular orbital study of the bonding in complexes of lithium with polynuclear aromatic hydrocarbons ... 389
Mukherjee, D., see Pal, S., et al. ... 125
Nakao, R., see Koga, T., et al. ... 211
Nath, S., see Sen, K. D. ... 139
Natiello, M. A., see Gavarini, H. O., et al. ... 171
Orendt, A. M., Facelli, J. C., Grant, D. M., Michl, J., Walker, F. H., Dailey, W. P., Waddell, S. T., Wiberg, K. B., Schindler, M., Kutzelnigg, W.: Low temperature ^{13}C NMR magnetic resonance in solids. 4. Cyclopropane, bicyclo[1.1.0]butane and [1.1.1]propellane ... 421
Pal, S., Prasad, M. D., Mukherjee, D.: A variational coupled cluster theory for closed shells using a propagator modification procedure ... 125
Pal, S.: Study of approximate coupled cluster methods for first-order static properties ... 379
Prasad, M. D., see Pal, S., et al. ... 125
Roos, B. O., see Wolinski, K., et al. ... 431
Ruedenberg, K., see Schmidt, M. W., et al. ... 69
Ruedenberg, K., see Valtazanos, P., et al. ... 471
Sadlej, A. J., see Wolinski, K., et al. ... 431
Schindler, M., see Orendt, A. M., et al. ... 421
Schmidt, M. W., Lam, B., Elbert, S. T., Ruedenberg, K.: Chemical binding and electron correlation in diatomic molecules as described by the FORS model and the FORS-IACC model ... 69
Schwarz, W. H. E., see Valtazanos, P.,et al. ... 471
Schwenke, D. W., see Brown, F. B., et al. ... 23
Sen, K. D., Nath, S.: A simple eigenvalue sum-density relationship for atoms ... 139
Shi, S., Miller, W. H.: A semiclassical model for intramolecular vibrational relaxion of local mode overtone in polyatomic molecules ... 1
Sinanoğlu, O.: New method for qualitative quantum chemical deductions on organic or inorganic molecules or clusters directly from structural or ORTEP diagrams ... 251
Somasundram, K., see Handy, N. C., et al. ... 87
Tomasi, J., see Cammi, R., et al. ... 271

Truhlar, D. G., see Brown, F. B., et al. ... 23
Valtazanos, P., Schwarz, W. H. E., Ruedenberg, K.: Electron difference densities and chemical bonding ... 471
Vener, M. V., see Ishenko, S. Ia., et al. ... 351
Waddell, S. T., see Orendt, A. M., et al. ... 421
Walker, F. H., see Orendt, A. M., et al. ... 421
Wang, F. E., see Chiu, Y.-N. ... 179
Wenchen, H., Wenjie, H.: A novel nomenclature of polycyclic aromatic hydrocarbons without using graph centre ... 301
Wenjie, H., see Wenchen, H. ... 301
Wiberg, K. B., see Orendt, A. M., et al. ... 421
Wolinski, K., Roos, B. O., Sadlej, A. J.: Polarized basis sets and the calculation of infrared intensities from nuclear electric shielding tensors ... 431
Zylka, C.: A note on the attainability of states by equalizing processes ... 363

Book reviews

Csizmadia, I. G.: Progress in theoretical organic chemistry. III. Molecular structure and conformation ... 335
Dugundji, J., see Ugi, I., et al. ... 249
Kopp, R., see Ugi, I., et al. ... 249
Lahmani, F.: Photophysics and photochemistry above 6 eV ... 420
Marquarding, D., see Ugi, I., et al. ... 249
McWeeny, R.: Coulsons Chemische Bindung ... 507
Ohtaki, H., see Tanaka, N., et al. ... 419
Perram, J. W.: The physics of superionic conductors and electrode materials ... 250
Schaefer III, H. F.: Quantum chemistry, the development of *ab initio* methods in molecular electronic structure theory ... 248
Tamamushi, R., see Tanaka, N., et al. ... 419
Tanaka, N., Ohtaki, H., Tamamushi, R.: Ions and molecules in solution ... 419
Ugi, I., Dugundji, J., Kopp, R., Marquarding, D.: Perspectives in theoretical stereochemistry ... 249
Wilson, S.: Electron correlation in molecules ... 247

Indexed in Current Contents

Subject Index

Ab initio wave functions 291
Adiabatic multi-step separation method 321
Asymmetry parameters 143
Atomic charge 221
Atomic charges 291
Atoms and molecules 379
Atoms in molecules 69

Barriers to migration 389
Basis sets 431
Basis set superposition error 271
Benzenoid hydrocarbons 107, 315
Bond angles 407
Bond energies 231
Bond index 337
Bond order 221
Bond polarity 211
Butadiene 101
1,3-Butadiene 57

Chaos-enhancing processes 363
Characteristic polynomials 107, 155
Charge transfer 389
Chemical bond 471
Chemical shift anisotropy 421
Classical valence bond theory 407
Clusters 251
Compact naming 315
Conical intersection 45
Convergence of the CI-expansion 445
Correlation cusp 445
Counterpoise corrections 271
Coupled cluster methods 379
Coupled cluster theory 125
Coupled oscillators 321
Covalent bond 471
Cut set 301
Cyclohexene conformations 101
Cyclopentadiene 101

Density-density correlation function 337
r_{12}-Dependent wave functions 445
Diatomic molecules 69
Diels-Alder transition state 101
Difference densities 471
Dipole moments 69
Directional moment of momentum 211
Dissociation curves 69

Eigenvalue problem 351
Electron correlation 69
Electron densities 471
Electron density 197
Electron momentum distribution 211
Electron transfer 159
Ethyl 57
Ethylene synchronism 101
(1/*Z*)-Expansion 445

Formaldehyde cation 57
Formaldimine 45
FORS/CASSGF 69

Graphical invariants 107
Graphite-lithium intercalates 389
Graphs 155
Graph theory 107

Hellmann-Feynman theorem 431
He-isoelectronic series 445
He-matrix 301
Hierarchy 321
Highly strained compounds 421
H_2O 431
Hydrogen bond 271
Hylleraas-CI 445
Hypervalency 231

Information theory 143
Infrared intensities 431
Interaction energy decomposition 271
Intramolecular hydrogen bond 351
Intramolecular vibrational relaxation 1
IPPP-INDO 171

Jahn-Teller distortion 285

Kekulé structure 301
Kinetic coupling model 1

LCAO-MO 179
Liquid metal 197
Lithium π complexes 389
Localized states 159
Local mode overtone absorption spectra 1
Löwdin analysis 221

Malonic dialdehyde 351
Many body theory 125
Metal clusters 179
Metalloproteins 159
Methoxy 57
Mode of rearrangements 155
Molecular properties 431
Molecular topology 101
Mulliken analysis 221
Multi-dimensional problem 321
Multireference configuration interaction calculations 23

Net populations 291
NMR couplings 171
Nodal increments 315
Non-bonding MO's 251
Non-pairwise additive potential surface 23
Numerical methods 351

Orbital population 221
f-Orbitals 179
Order structure of states 363
ORTEP 251
Overlap integrals 179

PAH characteristic graph 301
Perturbation-dependent basis sets 431
Perturbation series convergence 87
Photochemistry 45
Polarized basis sets 431
Polyhedra 143
Polynuclear aromatic hydrocarbons 389
Population analysis 231
Propagators 125
Proton hyperfine 57
P *spd* basis set 171

Qualitative quantum chemistry 251
Quantum chemical calculation of shielding tensors 421

Reduced wavefunctions 321
Regions of attainability 363

Second-order density matrix 337
Semiclassical perturbation approximation 1
Separatrix 285
Singlet biradical 285
Spectra 69
Spherical harmonics expansion 291
Spin densities 57
Static properties 379
Structural stability of a dynamical system 285
Surface profile 197
Symmetry 143
Symmetry orbitals 179
Syn-anti isomerization 45

The half-order ">" 363
Through-space 171
Total π-electron energy 315

Valence state energy 407
Valency 221
Valency changes 343
Vibrational-rotational scattering calculations 23

Water 407
Woodward-Hoffman reactions 343